# PAH Infrared Spectroscopy in the JWST Era

Completed Technology Project (2017 - 2019)

## Project Introduction

The extraordinary infrared instruments on the James Webb Space Telescope (JWST) will transform the field of cosmic spectroscopy. We propose to supply the astronomical community with theoretical and experimental spectra of a wide range of Polycyclic Aromatic Hydrocarbons (PAHs) and PAH clusters and to use our IR absorption spectra to calculate emission spectra that will be crucial in interpreting the new observational data. The Infrared Space Observatory and Spitzer Space Telescopes have shown that the mid-IR emission spectrum of the interstellar medium is dominated by strong bands at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 microns superimposed upon broad underlying plateaus generally attributed to PAHs, PAH clusters and very small grains. Despite the limited spectral and spatial resolution of these data, detailed analysis has revealed that each band is, in fact, a blend of multiple emission features. Subtle variations in the band blending can be detected even for spectra measured at different positions within a single astronomical source. These variations can be seen to arise from multiple PAH and PAH-related carriers that are each responding differently to the local physical conditions. The James Webb Space Telescope has near-IR and mid-IR instruments, NIRSpec and MIRI, with an extremely high spectral resolution, spatial resolution, and sensitivity that will revolutionize infrared astronomy. These instruments will provide spatial maps on a sub-arcsecond scale with an unprecedented level of spectral detail, allowing detailed study of the interrelationship of the individual components within each emission band. This will provide a critical insight into the molecular characteristics of the emitting species and their (photo)chemical evolution in space. Exploitation of these astronomical spectra requires fundamental data on potential emitting species that fully account for all astrophysically relevant materials. Over the last two decades, spectra of neutral and charged PAHs have been calculated using quantum theory. Due to computational limitations, this data set is biased towards smaller or highly symmetric species. In addition, continued analysis of the mid-IR emission bands by several recent Spitzer studies, has demonstrated that PAHs and PAH clusters with less symmetric structures containing “bay regions” are more important for understanding the IR emission bands than had previously been realized. The currently available infrared data set on less symmetric PAHs and PAH clusters is insufficient to exploit the astronomical data. Advances in computing power now allow spectra for a much wider range of species to be calculated. In support of the analysis of Spitzer data and the upcoming JWST mission, we therefore propose to calculate the 3-20 micron spectra of isolated as well as clustered neutral and charged PAHs containing up to 150 carbon atoms and with a wide range of compact structures and eroded structures with irregular shapes containing “bay regions”, “coves”, and “fjords”. These theoretical data will be validated by a dedicated laboratory study of PAH species and their clusters. These IR absorption spectra will be used to calculate emission spectra that can be directly compared to existing astronomical observations and that will be used to guide our quantum chemical and experimental studies on relevant species

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## Organizational Responsibility

**Responsible Mission Directorate:**

Science Mission Directorate (SMD)

**Responsible Program:**

Astrophysics Research and Analysis

## Project Management

**Program Director:**

Michael A Garcia

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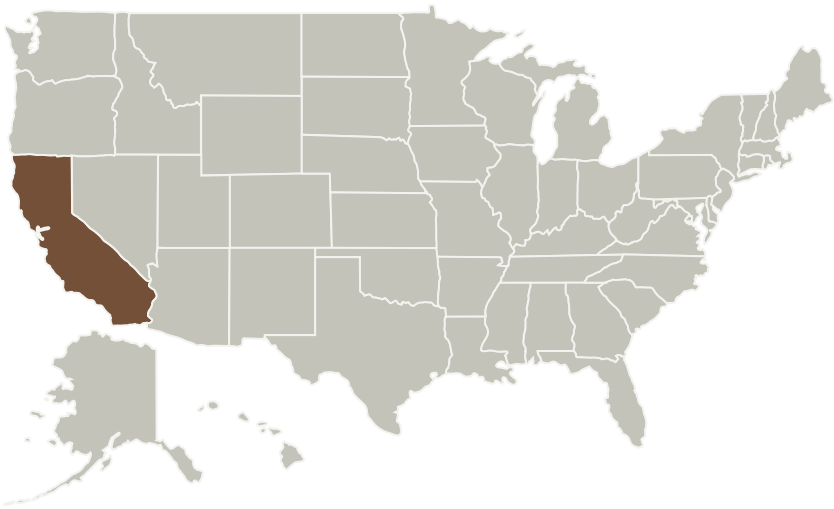
for support of Early Release Science proposals for JWST.

### Primary U.S. Work Locations and Key Partners



| Organizations Performing Work | Role | Type | Location |
|---|---|---|---|
| SETI Institute(SETI) | Supporting Organization | Academia | Moffett Field, California |

| Primary U.S. Work Locations |
|---|
| California |

## Project Management *(cont.)*

**Program Manager:**

Dominic J Benford

**Principal Investigator:**

Alessandra Ricca

**Co-Investigators:**

Xander G Tielens
Joseph E Roser
Barbara E Vance
Jean Chiar
Els Peeters

## Technology Areas

**Primary:**

- TX08 Sensors and Instruments
  - TX08.1 Remote Sensing Instruments/Sensors
    - TX08.1.1 Detectors and Focal Planes

## Target Destination

Outside the Solar System